cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(2-ethylhexyl) ester

Inchi: InChI=1S/C24H42O4/c1-5-9-13-19(7-3)17-27-23(25)21-15-11-12-16-22(21)24(26)28-18-

InchiKey: SVVBLKNHJWTATO-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CCCCC(CC)COC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-274.82	kJ/mol	Joback Method
hf	-947.09	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.088		Crippen Method
mcvol	348.740	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2510.00		NIST Webbook
tb	914.26	K	Joback Method
tc	1120.89	K	Joback Method
tf	478.46	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.48	J/mol×K	914.26	Joback Method
cpg	1208.56	J/mol×K	948.70	Joback Method
cpg	1226.06	J/mol×K	983.14	Joback Method
cpg	1242.01	J/mol×K	1017.57	Joback Method
cpg	1256.43	J/mol×K	1052.01	Joback Method
cpg	1269.37	J/mol×K	1086.45	Joback Method
cpg	1280.86	J/mol×K	1120.89	Joback Method
dvisc	0.0008462	Pa×s	478.46	Joback Method
dvisc	0.0003540	Pa×s	551.09	Joback Method

dvisc	0.0001815	Pa×s	623.73	Joback Method
dvisc	0.0001069	Pa×s	696.36	Joback Method
dvisc	0.0000696	Pa×s	768.99	Joback Method
dvisc	0.0000488	Pa×s	841.63	Joback Method
dvisc	0.0000362	Pa×s	914.26	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume